Los Alamos
NATIONAL LABORATORY
memorandum

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To/MS: ESH-6 Distribution
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Date: August 5, 1996

SUBJECT: NEWMENDF: A Prototype Multigroup Library with Self-shielded Cross Sections for ^{238}U and ^{240}Pu

I have completed the processing of a NEWMENDF multigroup library containing self-shielded cross sections for ^{238}U and ^{240}Pu in addition to the nuclides available on MENDF6. I have stored the new library on CFS under /x6data/working/esh6 and given read access to Kent Parsons (Z# 091475) and Doug O'Dell (Z# 076547). We can also transfer these to you on tape if needed.

Description of NEWMENDF

NEWMENDF is written in the standard random-access binary format for the Cray computers, please let me know if you need us to translate this to ASCII format for use with the DANT codes on your system. After you have used the prototype library for a number of calculations, we would like to discuss the choices for σ_o and further processing of other nuclides for ESH-6. The following new data are available on NEWMENDF:

Table 1: New Cross Section Data Available on NEWMENDF

Nuclide	σ_o	ZAID	Index #
94-Pu-240	infinite (10^{10})	94240.70	701
	10^5	94240.71	702
	10^4	94240.72	703
	10^3	94240.73	704
	10^2	94240.74	705
92-U-238	infinite (10^{10})	92238.70	710
	10^4	92238.72	712
	10^3	92238.73	713
	10^2	92238.74	714
	10^1	92238.75	715
	10^0	92238.76	716

The addition of self-shielding affects the data for the total, elastic, total and direct fission, (n,γ), and nubar*fission cross section data, as well as the scattering matrices. Prompt nubar remains the same as in MENDF6, and total nubar is not available on this library. Figures 1-10 show the total cross-section, total and direct fission, (n,γ), and nubar*fission data for ^{240}Pu and ^{238}U respectively.

Note that the *.70 data are ‘equivalent’ to the *.60 data on MENDF6 with the exception of differences due to processing. The new data represent NJOY processing with tighter tolerances for the thinning of the cross section data and the secondary energy distributions.   As you can see for Figures 11-14 , the new data for prompt and total chi as a function of energy are moderately different than that in MENDF6 for both nuclides. This is apparently the result of *not* thinning as much as was done for the production of MENDF6. There were no appreciable differences in the cross sections themselves between the two sets of data as illustrated in Figures 15-16 for the total cross section for both nuclides. One additional note, remember that the MENDF-type libraries contain prompt nubar data only.

Information on Production and QA of Data Library

As you are aware, we ran into some difficulties with the processing of the data with NJOY. Bob MacFarlane corrected the problems with the DTFR module of NJOY, and the nubar*fission cross sections are now correctly self-shielded. MacFarlane also corrected the self-shielding for the photon production data, but photon production data are not included as a part of MENDF6 or NEWMENDF at this time.

Once NJOY has created the DTF files, the code CKDTF.F is run to massage the data into the format necessary for a MENDF-type library. An example of such massaging is using the total and delayed nubar and chi data on the DTF files to construct the prompt nubar and chi data that the MENDF libraries require. Additionally, the MENDF format only allows for cross-sections for only 10 reactions, and therefore data for different reactions must sometimes be combined, though this is not the case for these two nuclides. Once the massaged DTF files were obtained, they were appended to the standard MENDF6 library using the code RANXS2.

The code CKDTF.F also does some QA in addition to the massaging of the DTF files from NJOY. The total fission cross section is compared with the sum of the partial fission cross sections, the total cross section is compared with the sum of all partials, the total and nubar*fission cross section edits are compared with the corresponding values from the P_o matrix, and the multiplicity implied from the P_o matrix is compared with the multiplicity implied by the sum of the individual edit reactions. Negative P_o cross sections are flagged and higher order P_n cross sections are examined to make sure they are not greater than the P_o values. Summary information for each group, including neutron and photon multiplicities and average secondary energies are printed to an output file.

In addition to examining the NJOY output for the DTF files, a number of additional tests are performed on the final library. The code CHECKMG.F reads in a random-access multigroup library, and for each nuclide and group, the code calculates two scattering cross sections. The first scattering cross section, sig1, is equal to the following

$$\mathrm{sig1} = \sigma_{el} + \sigma_{in} + 2*(n,2n) + 3*(n,3n)\,.$$

The second scattering cross section, sig2, is the sum of the outgoing P_o scattering matrix from the group of interest (G) and is calculated as follows:

$$\mathrm{sig2}_G = \sum_{G'} \sigma^o_{G\rightarrow G'} \quad .$$

The code also tries to include other reactions as necessary for sig1 where the edit cross sections contain additional information from other reactions. This is not the case for the two nuclides discussed here. In addition to these two quantities, diff=sig1-sig2 and delta=diff/sig2 are also calculated. All information is printed to an output file, and any value for delta$\geq 1\times10^{-4}$ is flagged.

The code COMPMG.F is used to compare two multigroup libraries. The code first compares the upfront information on each library such as the titles, energy boundaries, fluxes, velocities, and the chis. Any differences greater than 1×10^{-8} are printed. Next, the code then compares each identical ZAID on the two libraries, and any fractional differences greater than 1×10^{-8} are printed. Finally, for ZAIDs unique to a particular library, all cross section data will be printed. For P_n data, the sum of the scattering terms for each incident group and each P_n order are compared.

Distribution:
Doug O'Dell, ESH-6 MS F691
Kent Parsons, ESH-6 MS F691
Tom McLaughlin, ESH-6 MS F691
P. Soran, XTM MS B226
D. Shirk, XTM MS B226
R. Little, XTM MS B226
S. Frankle, XTM MS B226 (3 copies)
R. Seamon, XTM MS B226
N. Keen, XTM MS B226
J. Hendricks, XTM MS B226
R. Alcouffe, XTM MS B226
XTM files

Figure 1: Total Cross Section for Pu-240

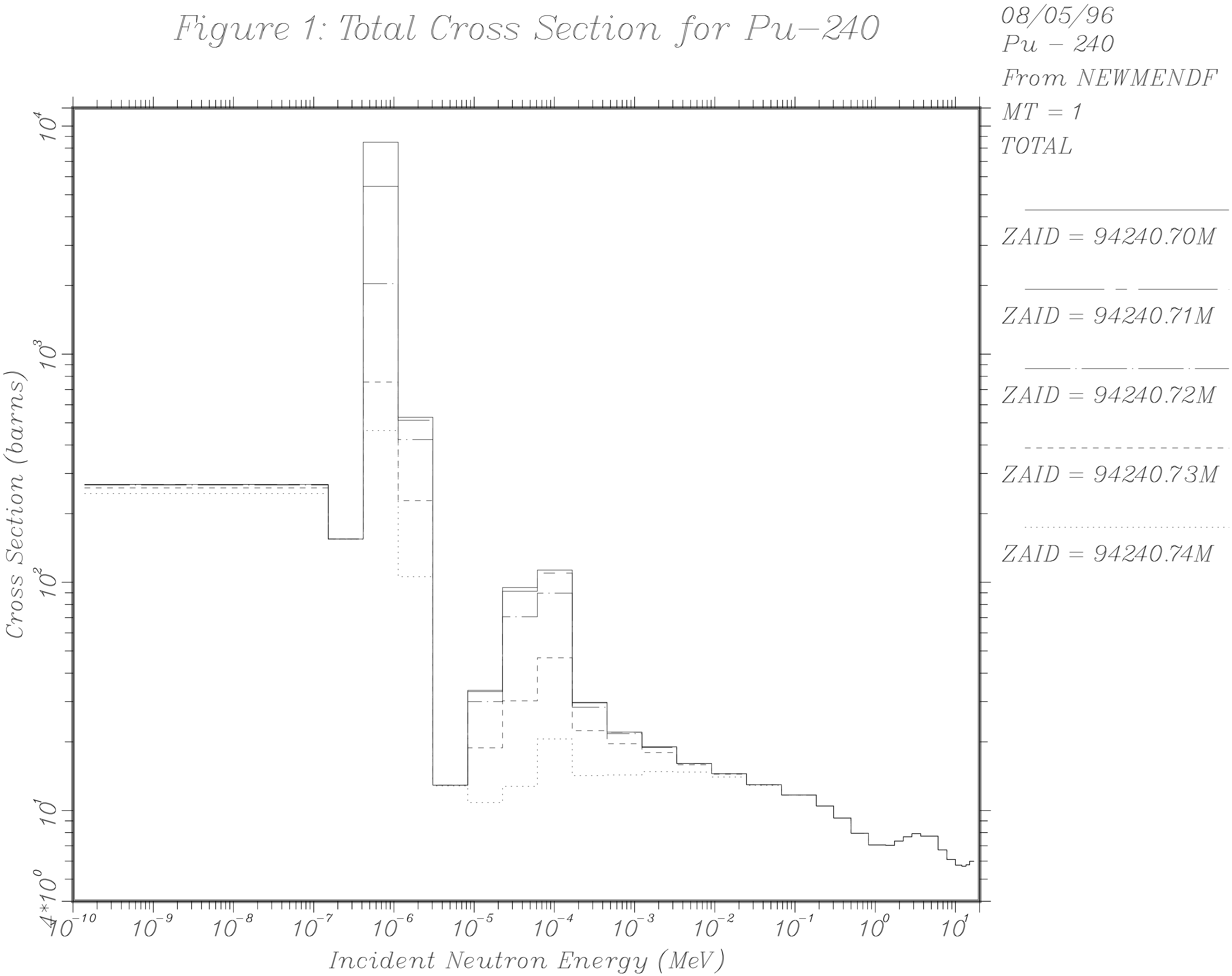
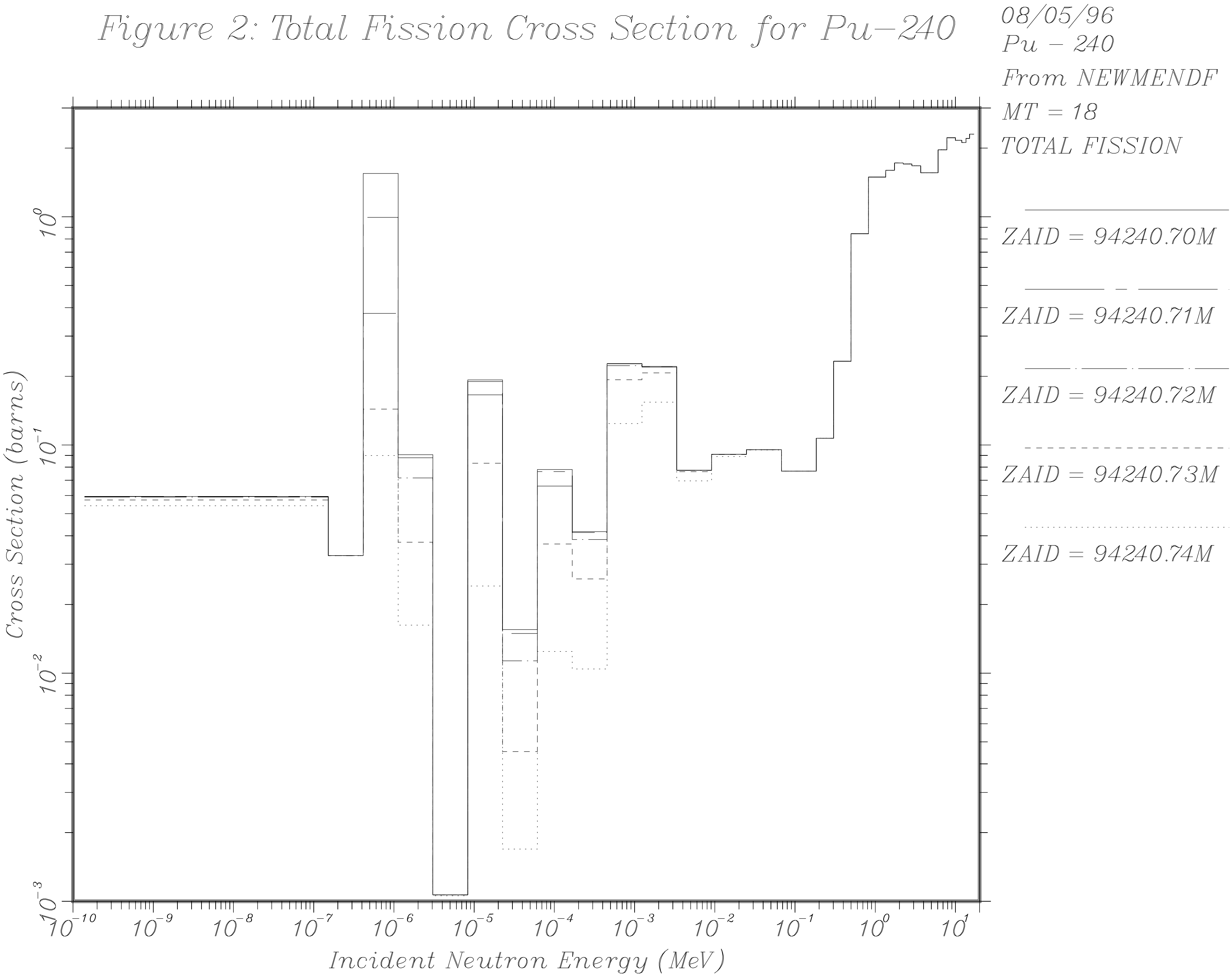


Figure 2: Total Fission Cross Section for Pu-240



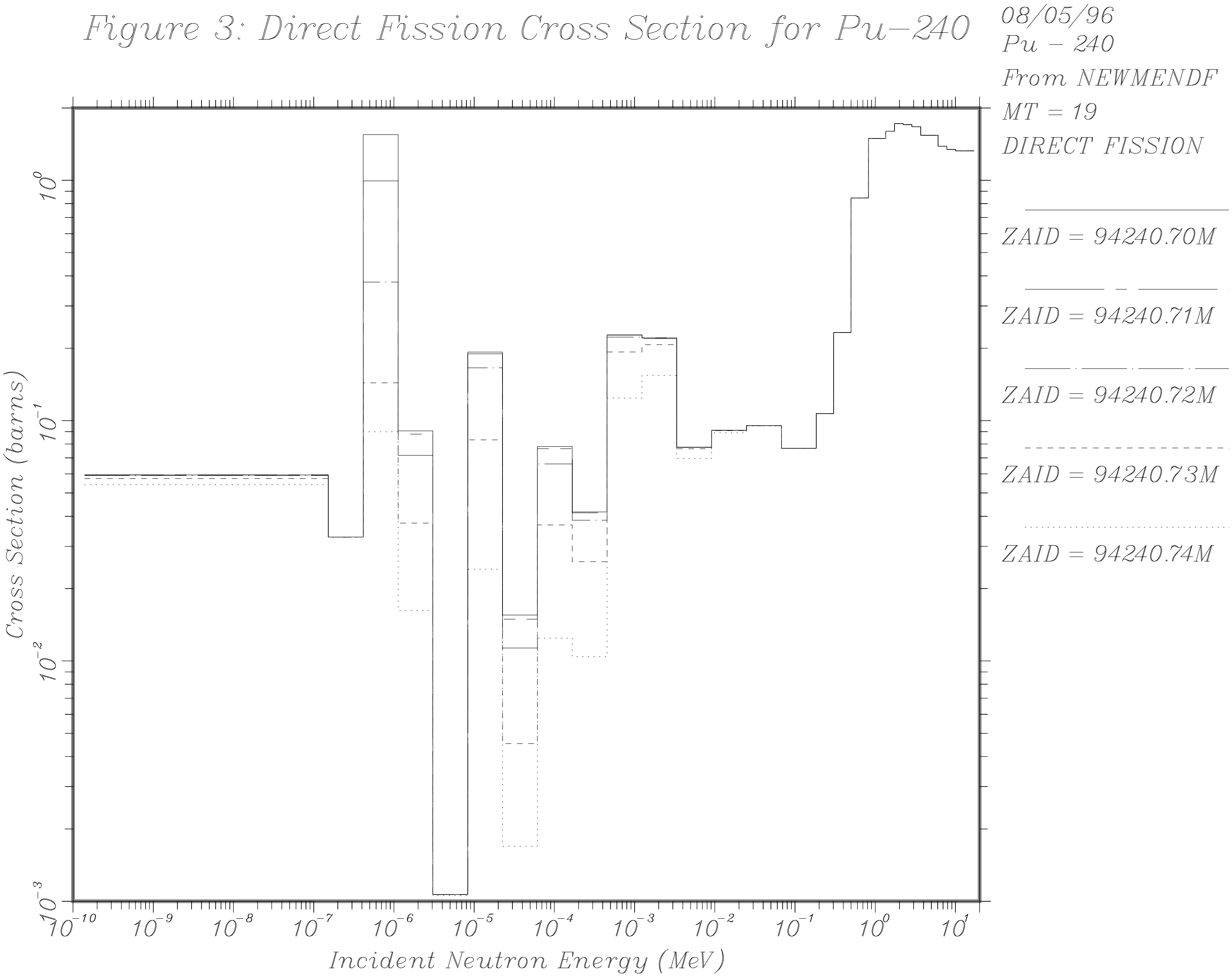


Figure 3: Direct Fission Cross Section for Pu-240
08/05/96
Pu - 240
From NEWMENDF
MT = 19
DIRECT FISSION
ZAID = 94240.70M
ZAID = 94240.71M
ZAID = 94240.72M
ZAID = 94240.73M
ZAID = 94240.74M
Cross Section (barns)
Incident Neutron Energy (MeV)

Figure 4: (n,gamma) Cross Section for Pu–240

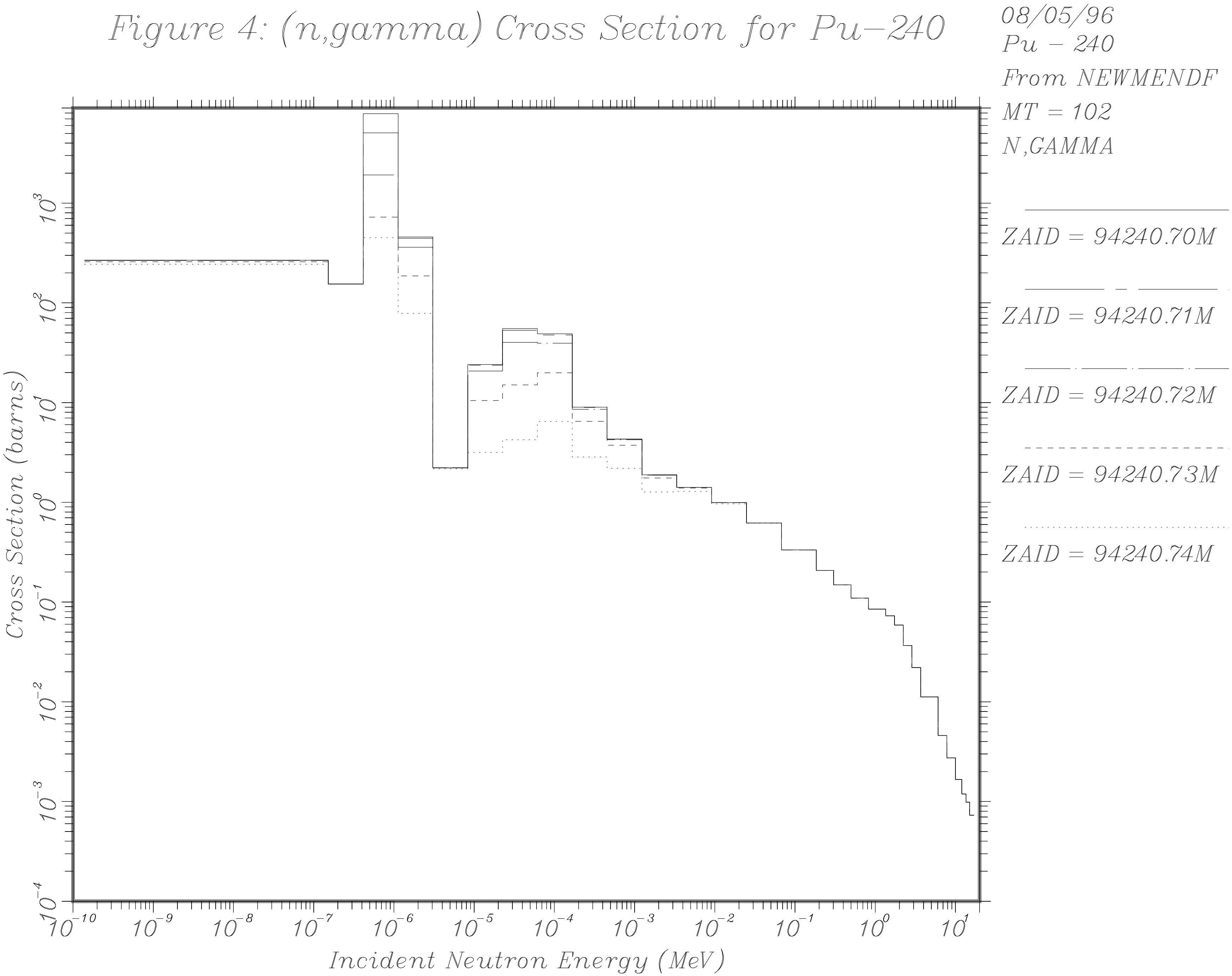


Figure 5: Nubar*Fission Cross Section for Pu-240

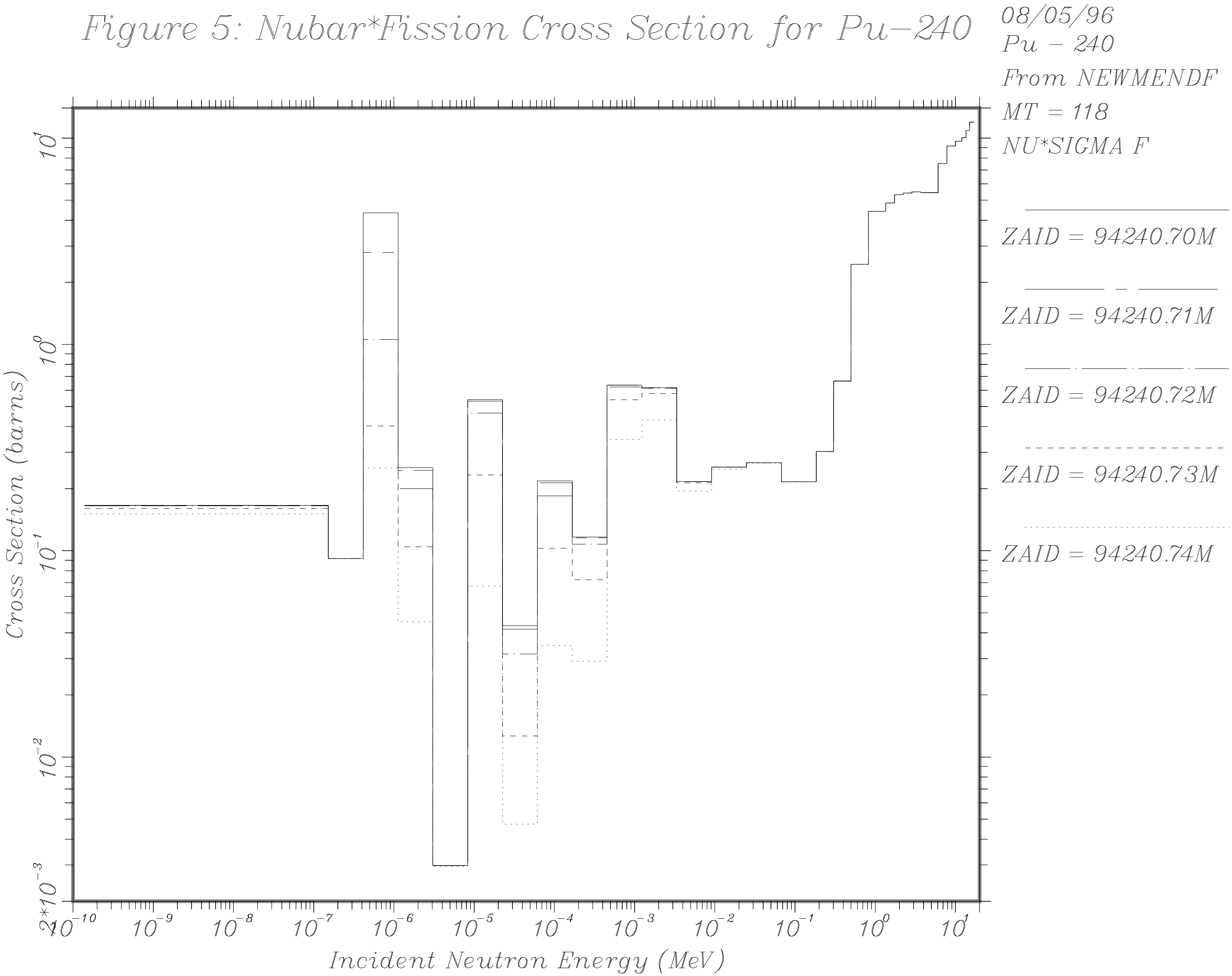
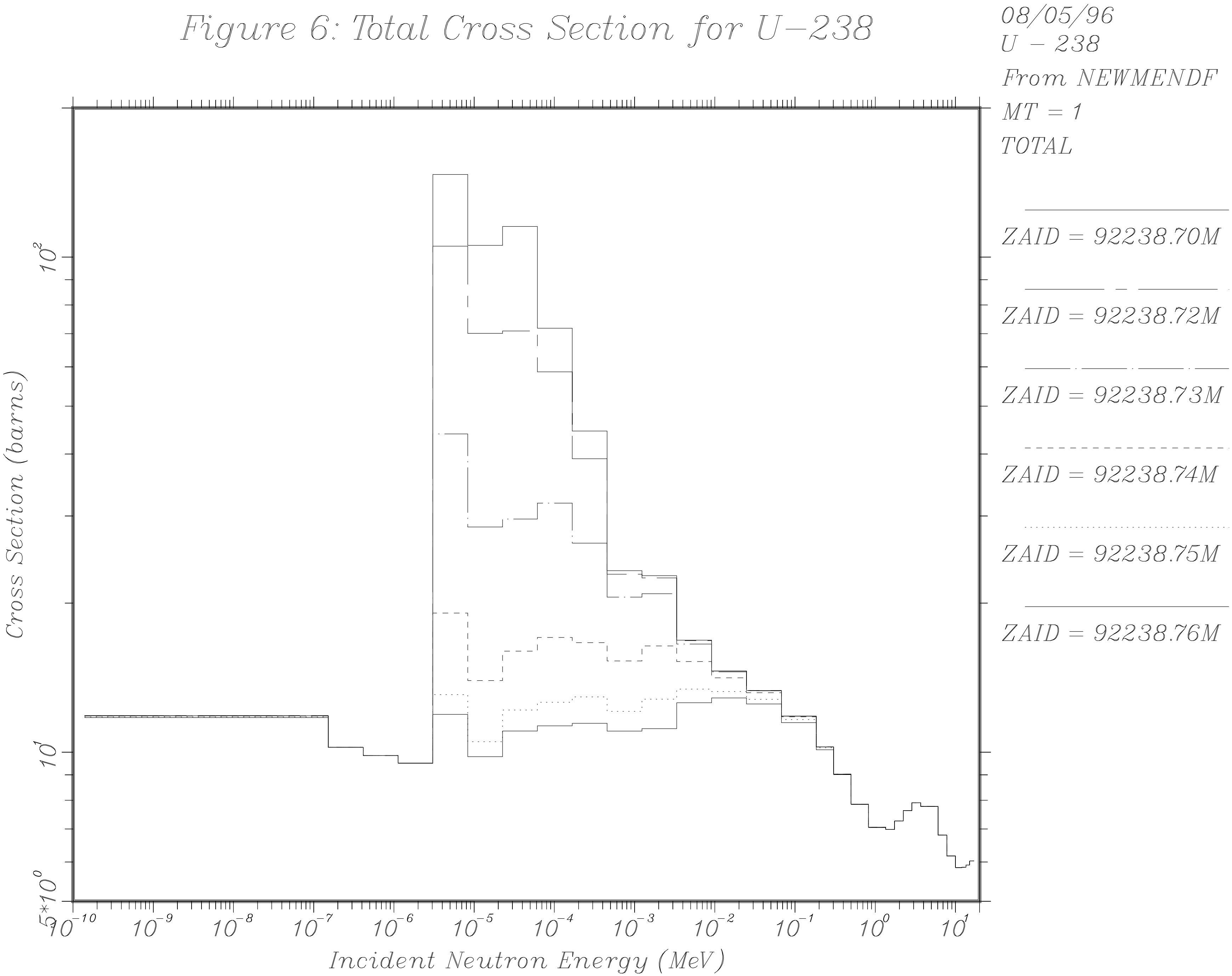


Figure 6: Total Cross Section for U−238



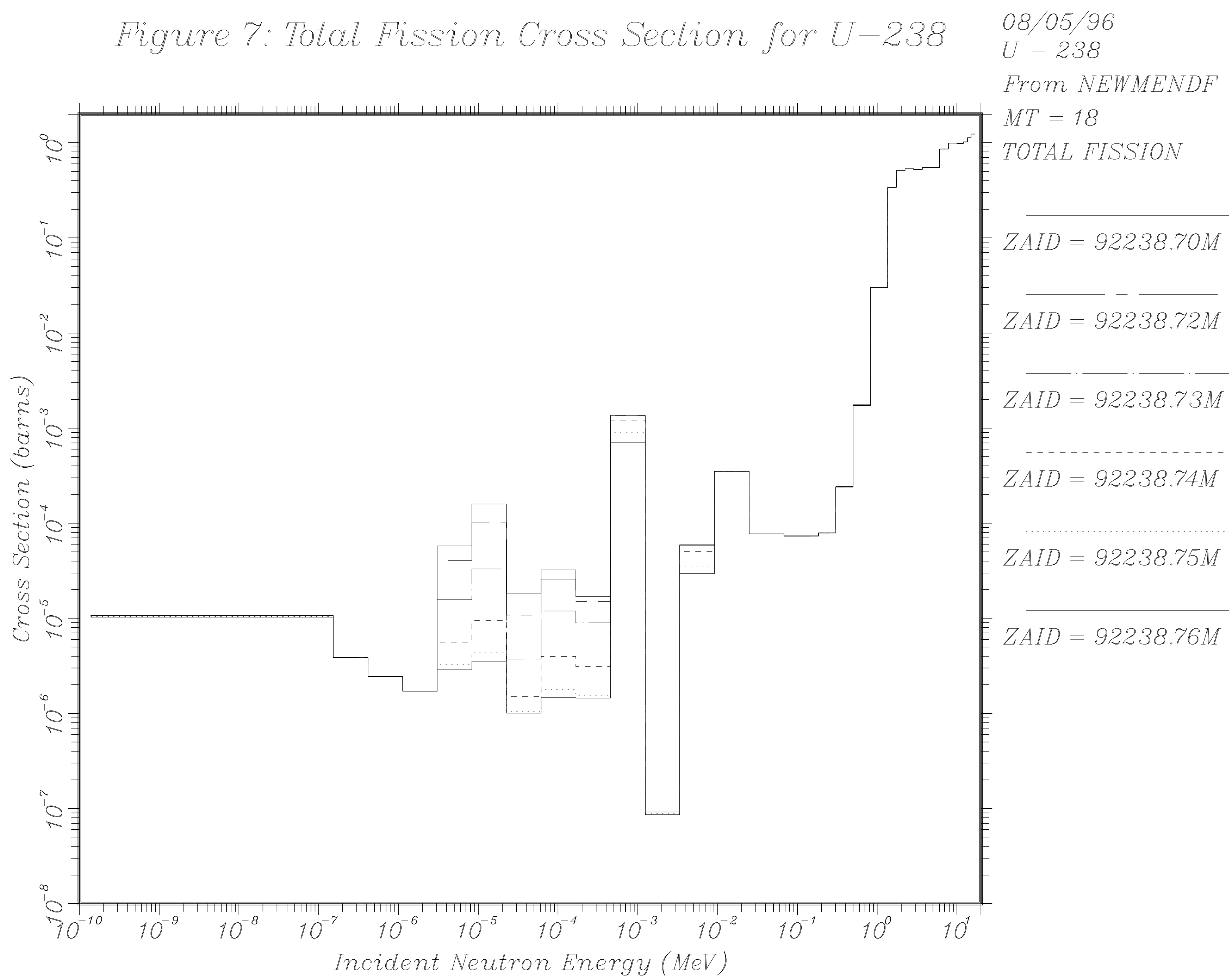


Figure 7: Total Fission Cross Section for U-238
08/05/96
U - 238
From NEWMENDF
MT = 18
TOTAL FISSION
ZAID = 92238.70M
ZAID = 92238.72M
ZAID = 92238.73M
ZAID = 92238.74M
ZAID = 92238.75M
ZAID = 92238.76M
Cross Section (barns)
Incident Neutron Energy (MeV)
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

Figure 8: Direct Fission Cross Section for U−238

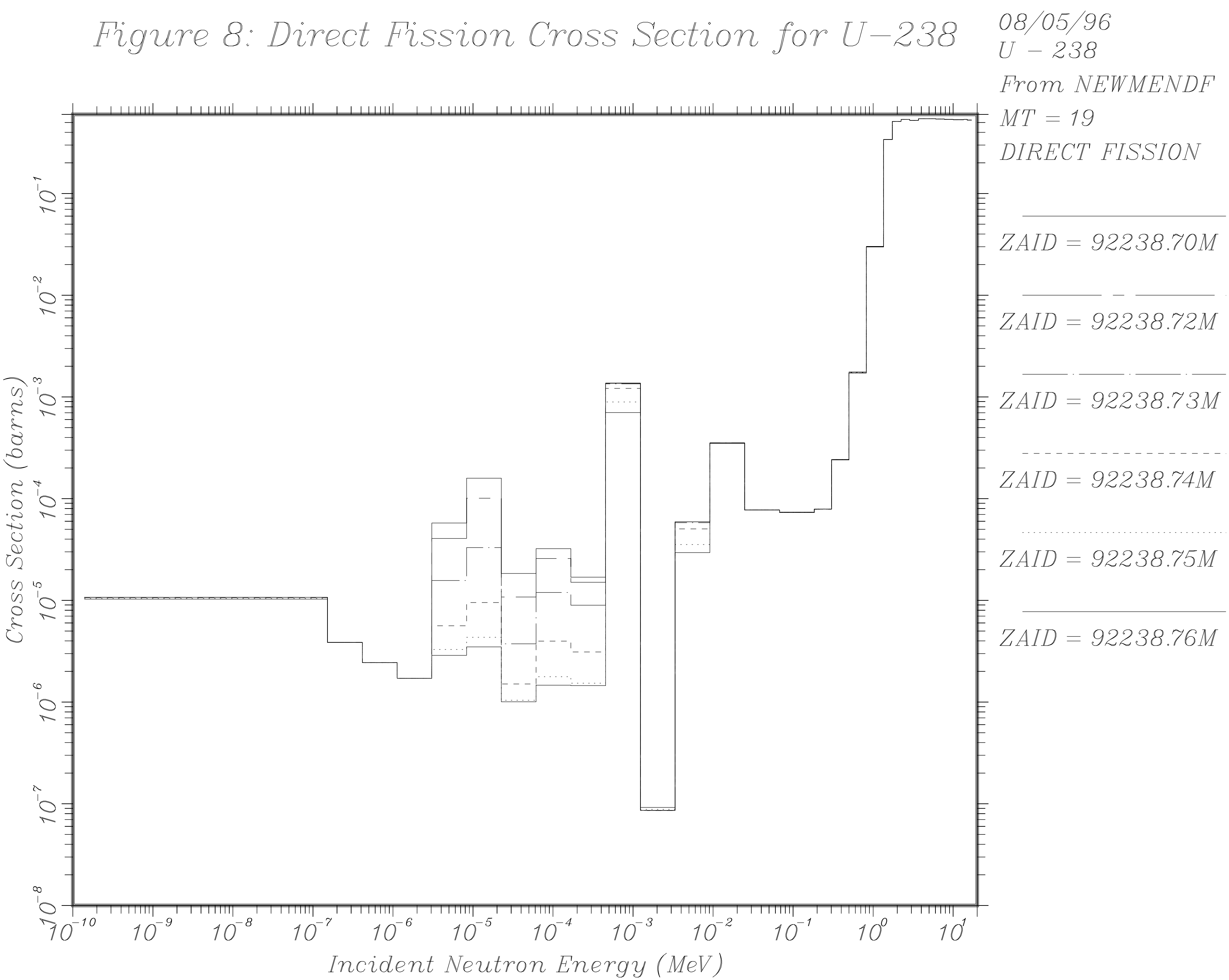


Figure 9: (n,gamma) Cross Section for U–238

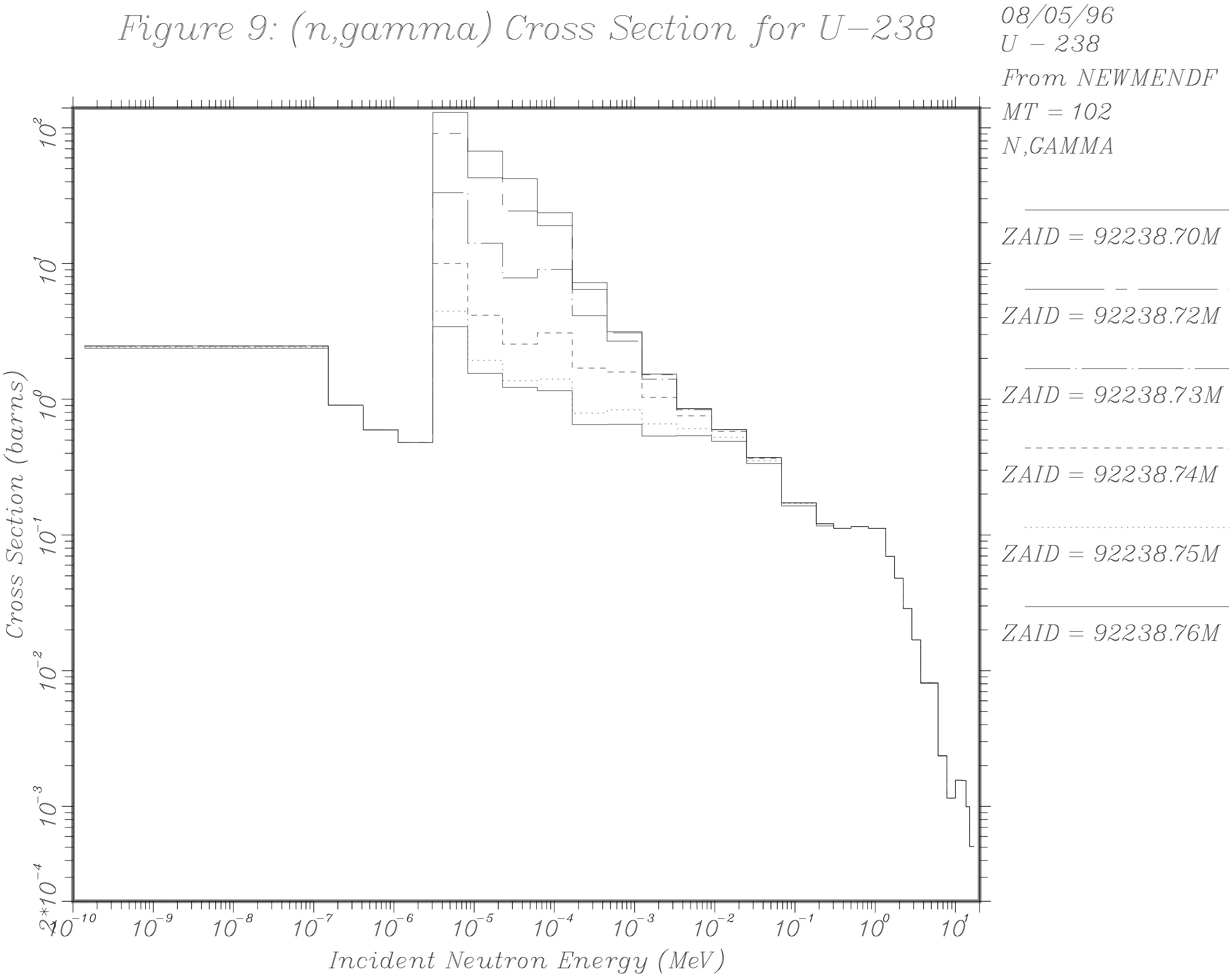


Figure 10: Nubar*Fission Cross Section for U-238

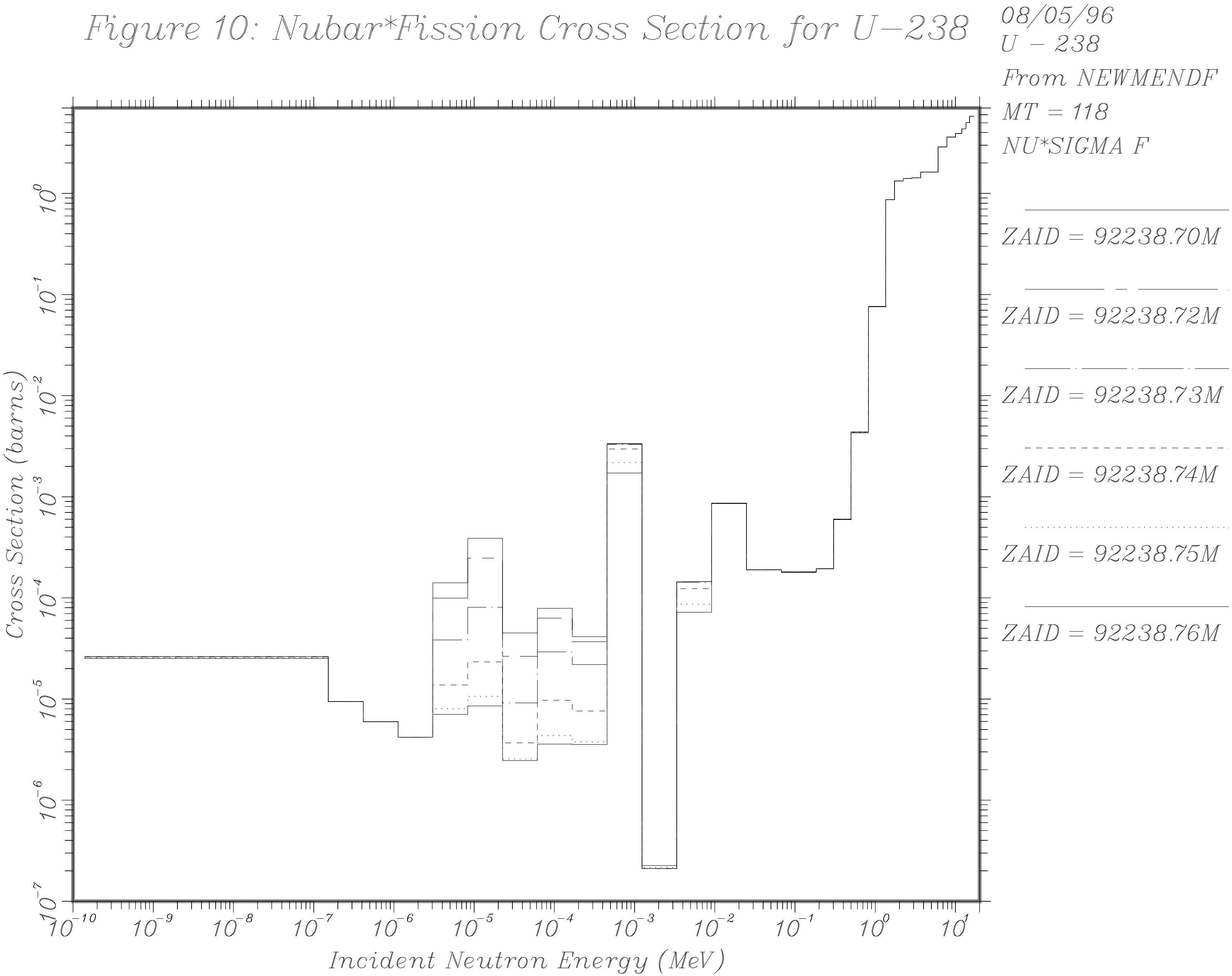


Figure 11: Prompt Chi for Pu–240

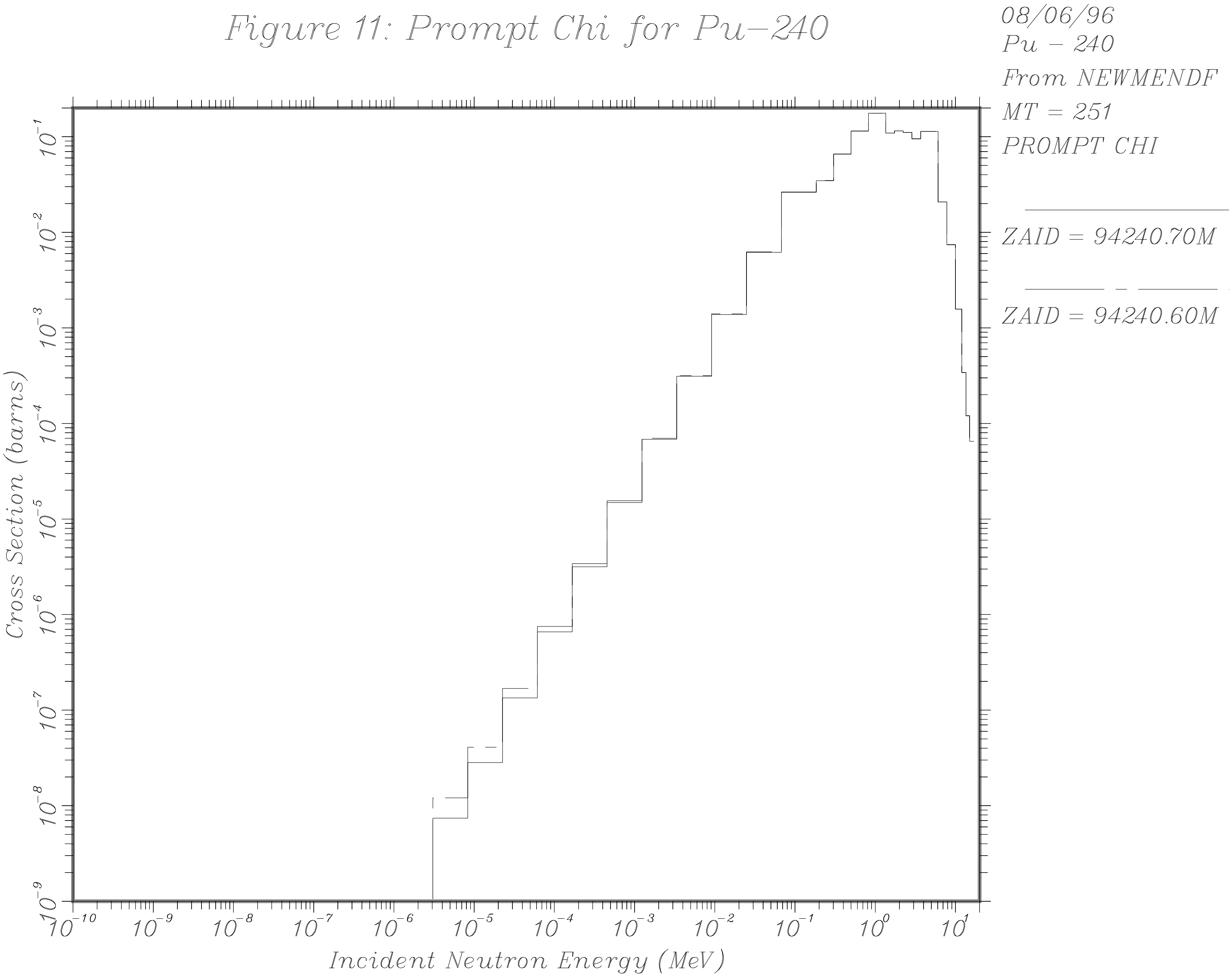


Figure 12: Total Chi for Pu–240

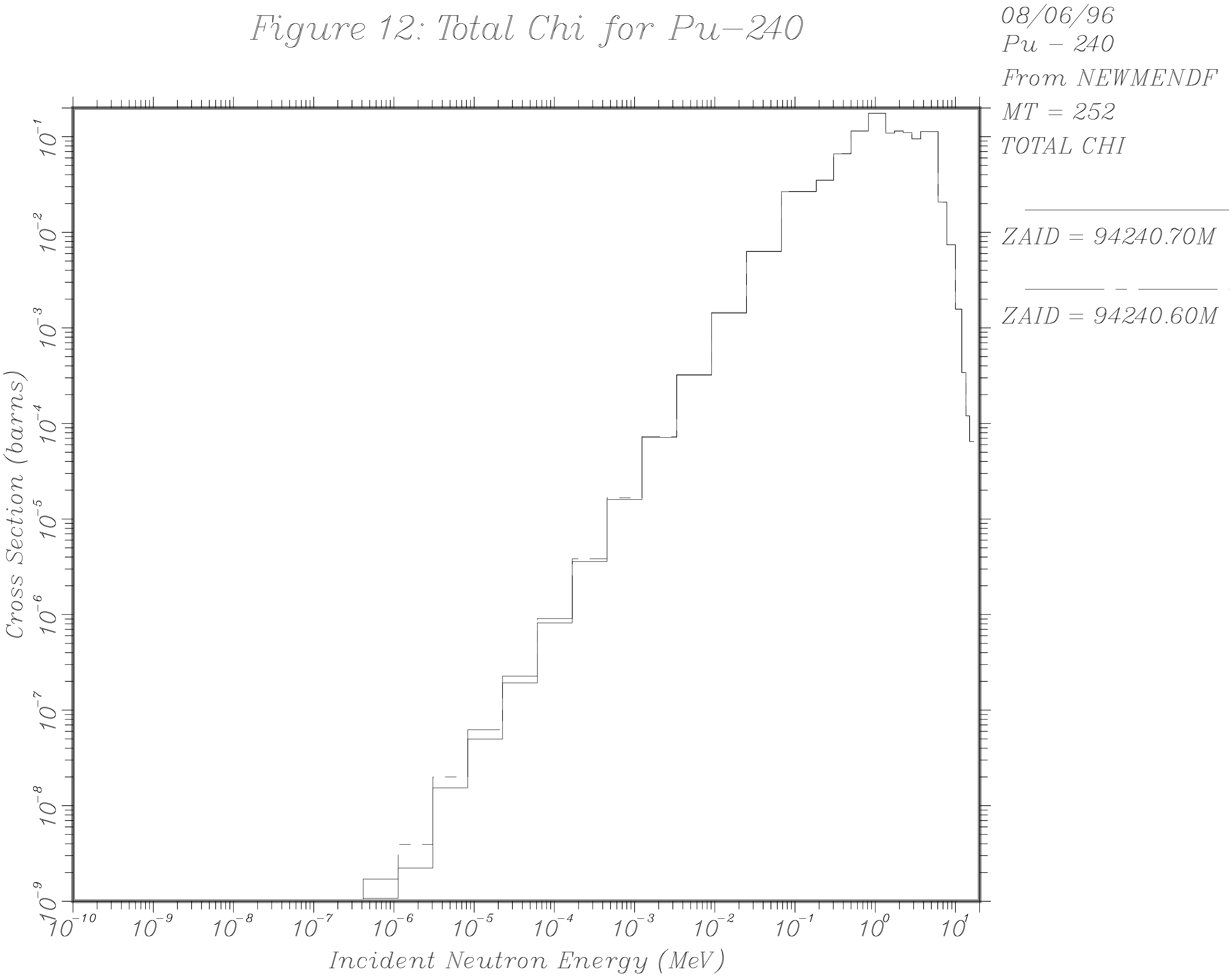


Figure 13: Prompt Chi for U−238

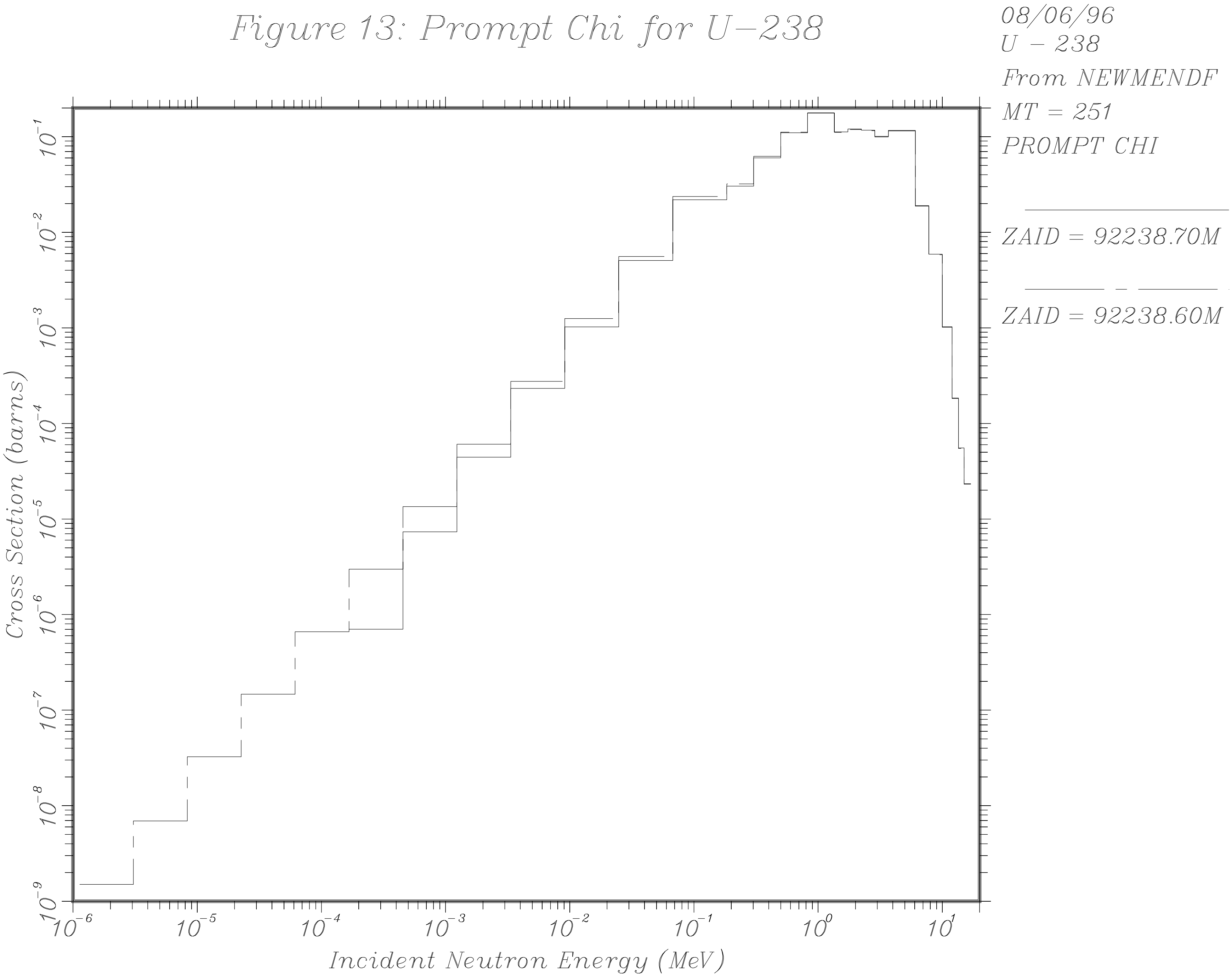
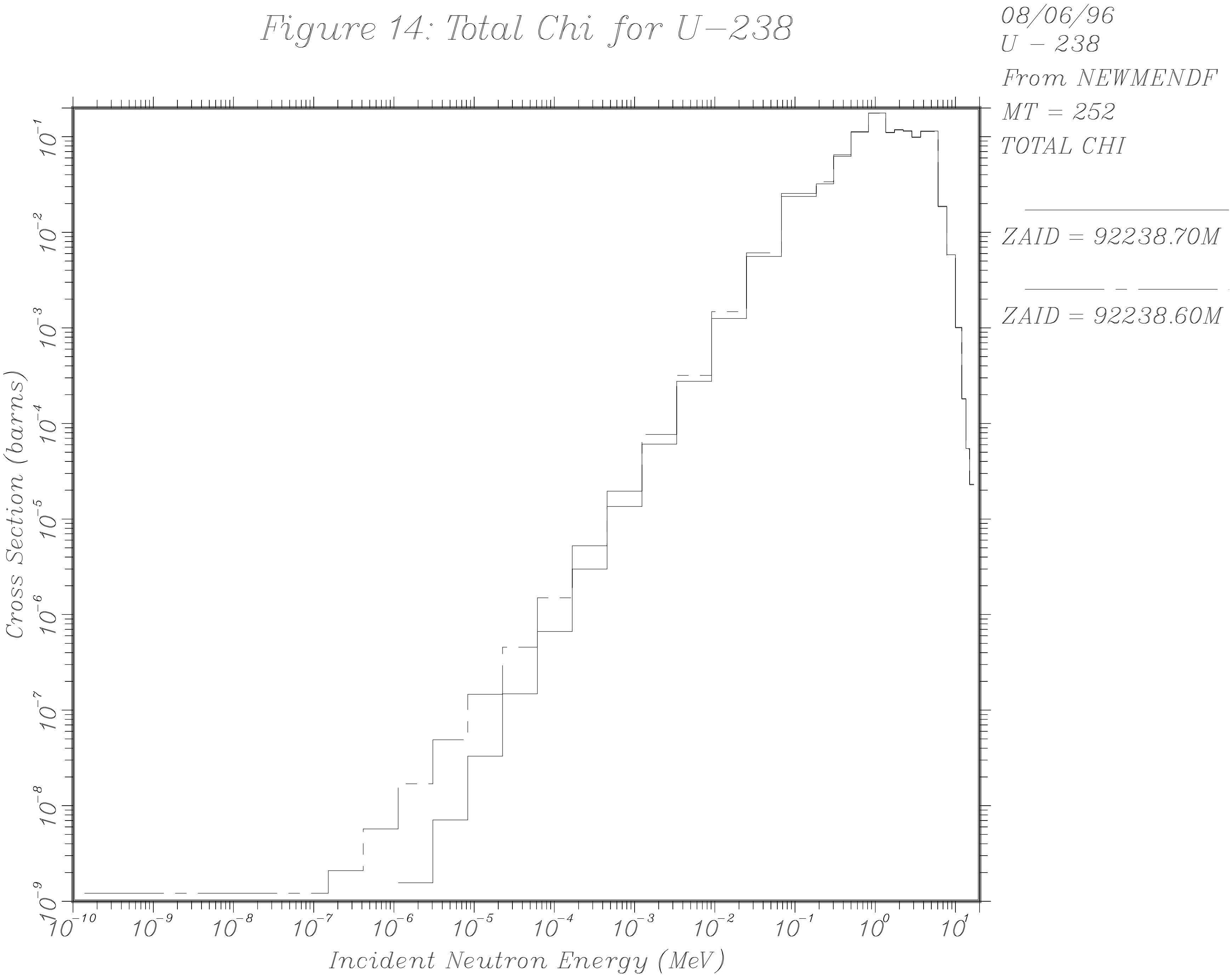


Figure 14: Total Chi for U-238



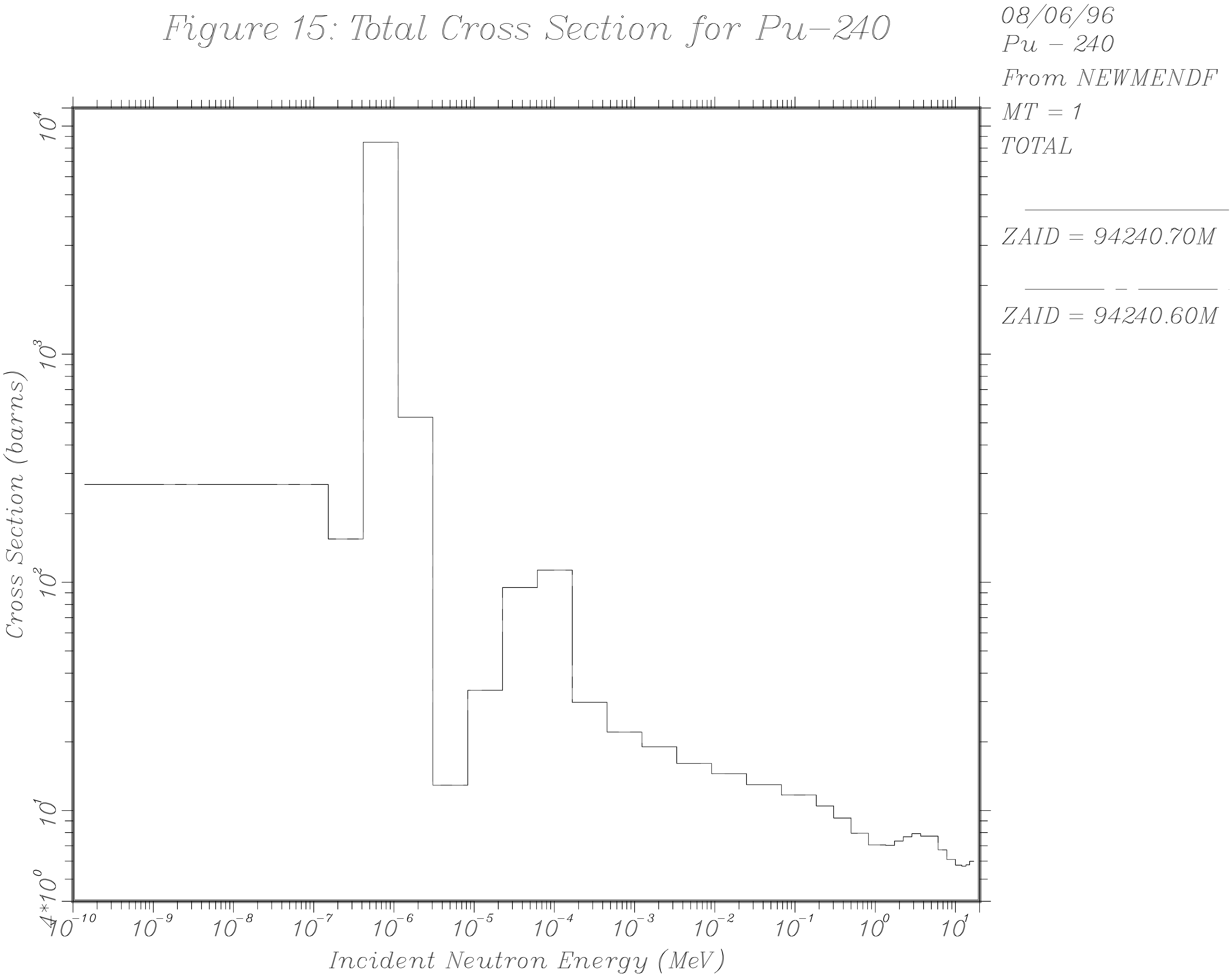


Figure 15: Total Cross Section for Pu-240
08/06/96
Pu - 240
From NEWMENDF
MT = 1
TOTAL
ZAID = 94240.70M
ZAID = 94240.60M
Cross Section (barns)
Incident Neutron Energy (MeV)

Figure 16: Total Cross Section for U−238